Hexanedioic acid, 2,2,3,3,4,4,5,5-octafluoro-

336-08-3 | DTXSID4059833

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.85

Global applicability domain: Outside

Local applicability domain index: 1.93e-01

Confidence level: 8.54e-01

Nearest Neighbors from the Training Set

Image not found
4-Amino-5-hydroxy-2,7-naphthalenedisulfonic acid monosodium salt
Measured: 2.88
Predicted: 2.48

Image not found
7-Amino-4-hydroxynaphthalene-2-sulfonic acid
Measured: 2.40
Predicted: 4.77

Image not found
6-Amino-4-hydroxynaphthalene-2-sulfonic acid
Measured: 4.07
Predicted: 4.77

Image not found
2-Amino-5-methylbenzenesulfonic acid
Measured: 3.98
Predicted: 6.29